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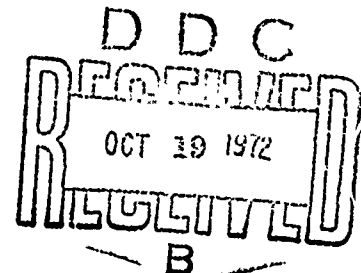
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## ABSTRACT

The problem treated in this paper is that of the evaluation of pressure waves that can be generated by clouds of explosive gas-air mixtures in a free atmosphere which is initially at a uniform state. The particular subject of this study is concerned with the final stage of the process when, following ignition and initial flame acceleration, the flame acquires the steady state of a constant velocity deflagration. Under the assumption of point, line or plane symmetrical geometry, the flow field is then self-similar. Theoretical results describing such flow fields are presented and numerical solutions, obtained for a representative case corresponding to a hydrocarbon-air mixture at normal atmospheric conditions, are given.

## INTRODUCTION

When an explosive gas-air mixture in an unconfined space is ignited at the center, either a flame or a detonation can be, at first, initiated, depending on the power density of the ignition energy. Under normal circumstances the former will then accelerate reaching soon a steady state of propagation, while the latter will most likely decay - a process accompanied by the gradual separation of the reaction zone from the shock front.

Such phenomena have been studied initially with reference to spherical detonations, by Manson <sup>(1)</sup>, Freiwald and Ude <sup>(2)</sup>, Zel'dovich et al. <sup>(3)</sup> and Leonas <sup>(4)</sup>. More recently, the knowledge in this field of study has been greatly enhanced as a consequence of the availability of modern experimental techniques, notably the use of the focused giant-pulse laser beam for ignition, as exemplified by the work of Lee <sup>(5)</sup>, and the application of high-frequency response pressure transducers combined with high resolution optical recording techniques, as illustrated by the studies of Soloukhin and Oppenheim <sup>(5)</sup>.

In both cases of ignition, whether it results in a flame or produces initially a detonation wave, the most likely eventual outcome of combustion in air is the establishment of a steady propagation state where the flame moves at a constant speed, acting, in effect, as a deflagration that leaves behind products at rest and generates ahead a pressure wave which, under proper geometrical conditions, acquires the character of a self-similar blast wave. It is the analysis of this case that forms the objective of this paper.

Such flow fields were studied by Taylor <sup>(6)</sup>, Sedov <sup>(7)</sup> and Shiken <sup>(8)</sup>, and discussed in the text of Courant and Friedrichs <sup>(9)</sup>. The analysis presented here follows, in essence, the technique of the above references; the formulation is, however, modified to take advantage of the simplifications that can be obtained as a consequence of our recent studies on the fundamental properties of blast waves <sup>(10,11)</sup>. The results are worked out in detail to yield a full description of the pressure wave that can be formed by a cloud of a hydrocarbon-air mixture. The possible effects of

geometry are taken into account by the consideration of either point-, line-, or plane-symmetrical motion. In free space the most probable shape the wave may take should be encompassed by the point- and line-symmetrical geometry, so that the physically realizable case should be bounded by these two solutions.

## PROBLEM

The time-space wave diagram of the system is presented in Fig. 1, the coordinates  $t$  and  $r$  being measured from the origin where all wave fronts intersect. The medium into which the leading wave front propagates, state (1), as well as the products of combustion behind the flame, state (4), are considered to be at rest. The flow field to be determined is self-similar, so that the trajectories of both the deflagration and the front discontinuity are straight lines, while the gasdynamic parameters remain invariant along similarity lines  $x \equiv r/r_2$ . With reference to Fig. 1, the continuous self-similar flow field is thus associated with the change of state from (2) to (3). An equivalent flow field can be generated by a piston whose path is also shown on this diagram. It is, in fact, such a piston-driven wave that formed the objective of the first paper of Taylor<sup>(6)</sup> in the subject of blast waves.

The problem is to determine the space profiles of the gasdynamic parameters, i.e., the pressure,  $p$ , density,  $\rho$ , temperature,  $T$ , and particle velocity,  $u$ , that would be established at any point in space in a combustible mixture giving rise to a deflagration front propagating into the medium immediately ahead of it at a given burning speed,  $S$ . Both the deflagrations associated with a pressure drop, as prescribed by the appropriate Hugoniot curve, as well as constant pressure deflagrations are considered in the analysis.

In a self-similar flow field each particle undergoes the same thermodynamic process. This is represented on the pressure-specific volume diagram in Fig. 2. After compression by the shock front from state (1) to state (2) represented by a point lying on the Rankine-Hugoniot curve, RH, the particle undergoes an isentropic compression in the blast wave to state (i) immediately ahead of the deflagration which, in turn, yields state (4) specified by a point lying on the appropriate Hugoniot curve, H. The latter can be either associated with a pressure drop terminating at state (j), or it can correspond to a constant pressure process ending at state (i).

## SOLUTION

The self-similar flow field of a blast wave can be described most concisely in terms of the following reduced parameters:

$$F \equiv \frac{t}{r\mu} u \quad \text{and} \quad Z \equiv \left( \frac{t}{r\mu} a \right)^2 \quad \text{where} \quad \mu \equiv \frac{t_2}{r_2} w_2 \quad (1)$$

$a$  is the local velocity of sound, while, with reference to Fig. 1,  $w_2 = dr_2/dt$ .

The reduced parameters represent the phase plane coordinates of the problem, so that its solution is obtained, in essence, by determining the appropriate integral curve which prescribes  $Z = Z(F)$ , subject to some specific boundary conditions. The latter are given, on one side, by the Rankine-Hugoniot relations across the shock front and, on the other, by the jump conditions across the deflagration front, yielding zero particle velocity in the burnt gas region immediately behind it. The condition of  $F = 1$  corresponds to the state at the piston face since then, at  $t = t_2$ , one obtains  $xw_2 = u$ , i.e., the piston velocity,  $xw_2$ , coincides with the particle velocity,  $u$ . In our notation, under such circumstances  $x = x_p$  while  $u = u_p$ .

For a blast wave whose front propagates at a constant velocity,  $\mu = 1$ . If the state of the undisturbed medium is uniform, while the substance is a perfect gas with constant specific heats, the conservation equations for such self-similar blast waves can be reduced to a single differential equation governing the solution, namely: <sup>(10)</sup>

$$\text{where} \quad \frac{d \log Z}{d \log F} = \frac{2D + j(\gamma-1)(1-F)F}{D + jZ} \quad (2)$$

$$D \equiv Z - (1-F)^2$$

while  $j = 0, 1, 2$  for the plane-, line-, and point-symmetrical geometry, respectively, and  $\gamma$  is the specific heat ratio.

Once the integral curve in the phase plane is known, the solution is completed by the quadrature

$$\frac{d \log x}{d \log F} = - \frac{D}{D + jZ} \quad (3)$$

while the gas dynamic parameters of the flow field are determined from the algebraic relations

$$u = w_2 x F \quad (4)$$

and, since the flow is isentropic,

$$\frac{T}{T_2} = \left( \frac{a}{a_1} \right)^{\frac{1}{\gamma}} = \left( \frac{\rho}{\rho_1} \right)^{\frac{\gamma-1}{\gamma}} = \left( \frac{p}{p_1} \right)^{\frac{\gamma-1}{\gamma}} = x^2 \frac{Z}{Z_1} \quad (5)$$

At  $F = 1$  Eqs. (2) and (3) become simply:

$$\frac{d \log Z}{d \log F} = \frac{2}{j+1} \quad (6)$$

$$\frac{d \log x}{d \log F} = - \frac{1}{j+1} \quad (7)$$

representing then also the governing differential equations for the plane-symmetrical case of  $j = 0$ . The solution in this case is thus obtained immediately by integration, giving

$$Z = Z_p F^2 \quad (8)$$

and

$$x = x_p F^{-1} \quad (9)$$

where  $Z_p = Z_{@F=1}$  and  $x_p = x_{@F=1}$ .

The solution to the problem is given in terms of a family of integral curves on the phase plane for which  $Z$  and  $F$  are the coordinates. Each curve corresponds to a fixed value of  $Z_p$  and  $X_p$ . They are shown for the case of  $\gamma = 1.3$ , on Fig. 3, labeled in terms of  $\zeta \equiv \delta Z_p$ , for spherical, cylindrical and plane flow fields corresponding, respectively, to  $j = 2, 1$  and  $0$ .

The curves were obtained by the numerical integration of Eq. (2) or, for  $j = 0$ , directly from Eq. (8), starting from the conditions at the piston face, that is  $F = 1$  and  $Z = Z_p = \zeta/\delta$ . They were terminated at the shock front whose phase plane coordinates are given by

$$F_2 = \frac{2}{\delta+1} (1-y)$$

and

$$Z_2 = \frac{2(\delta-1)}{(\delta+1)^2} \left( \frac{2\delta}{\delta-1} - y \right) \left( \frac{\delta-1}{2} + y \right) \quad (10)$$

where  $y \equiv a_1^2/W_1^2 = 1/M^2$ . Eliminating the latter from Eqs. (10) and (11) one obtains for the locus of end points

$$Z_2 = \frac{\delta-1}{2\delta} (1-F_2) \left( \frac{2}{\delta-1} + F_2 \right) \quad (11)$$

representing the equation of the Rankine-Hugoniot curve in the phase plane. The corresponding initial condition is that of a quiescent atmosphere ahead of the wave, that is

$$F_1 = 0$$

and

$$Z_1 = \frac{a_1^2}{W_1^2} = y \quad (12)$$

while the change of the gasdynamic parameters across the front is specified in terms

of the following shock relations:

$$\begin{aligned}\frac{p_2}{p_1} &= \frac{\delta-1}{\delta+1} \left( \frac{2\gamma}{\delta-1} - \gamma \right) \\ \frac{\rho_2}{\rho_1} &= \frac{\delta+1}{\delta-1+2\gamma} \\ \frac{T_2}{T_1} &= \frac{Z_2}{Z_1} = \frac{2(\delta-1)}{(\delta+1)^2} \left( \frac{2\gamma}{\delta-1} - \gamma \right) \left( \frac{\delta-1}{2} \frac{1}{\gamma} + 1 \right)\end{aligned}\tag{13}$$

For weak waves the Mach number of the front approaches unity and there arises a basic difficulty in the integration of the differential equation governing the structure of the blast wave. This is due to the particular property of the singularity of the point  $F=0$ ,  $Z=1$  which lies at the intersection of the Rankine-Hugoniot curve with the  $F=0$  axis, corresponding to the condition of  $M=1$  at the front<sup>(10)</sup>. The problem is caused by the fact that the integral curves representing the blast wave structure intersect the Rankine-Hugoniot curve at a positive slope that becomes larger for weaker waves, while they have to approach the singularity at  $F=0$  with an infinitely negative slope. The consequent rapid change in the derivatives produces queer numerical results which led Taylor<sup>(6)</sup> initially to the belief that there may be a lower bound to the solution corresponding to the condition that  $X$  cannot be smaller than a certain value, somewhat between 0.4 and 0.5.

Actually, as it has been indeed observed by Taylor<sup>(6)</sup>, when the front Mach number approaches unity, the problem is governed by the acoustic wave equation and, as it will be demonstrated here, there exists a continuous transition between the acoustic and blast wave domains, so that, in fact, the weak limit does not exist and  $X$  can be as small as one pleases.

The acoustic wave is described in terms of the velocity potential,  $\phi(r,t)$ , which satisfies the equation

$$\frac{\partial^2 \phi}{\partial t^2} = \frac{a_1^2}{r^j} \frac{\partial}{\partial r} \left( r^j \frac{\partial \phi}{\partial r} \right)\tag{14}$$

and is related to the particle velocity and pressure, respectively, as follows

$$\left. \begin{aligned} u &= -\frac{\partial \phi}{\partial r} \\ p - p_1 &= \rho_1 \frac{\partial \phi}{\partial t} \end{aligned} \right\} \quad (15)$$

Introducing the similarity variable  $X = \frac{r}{a_1 t}$ , and assuming for the potential the functional form  $\phi(r, t) = t f(X)$ , Eq. (14), is transformed into an ordinary differential equation

$$X(1-X^2) f'' + j f' = 0 \quad (16)$$

while Eq. (15) yields

$$u = -\frac{1}{a_1} f'(X)$$

and

$$\frac{p - p_1}{\rho_1} = \frac{j}{a_1^2} [f(X) - X f'(X)] = j \left[ \frac{f(X)}{a_1^2} - \frac{u(X)}{a_1} X \right] \quad (17)$$

Integrating Eq. (16), subject to the boundary conditions at the piston face where

$$u = u_p = a_1 X_p = -\left(\frac{\partial \phi}{\partial r}\right)_{r=r_p} = -\frac{1}{a_1} f'(X_p) \quad (18)$$

and at the front where

$$p = p_1 \quad \text{at} \quad r_2 = a_1 t \quad (19)$$

one obtains

$$F(X) = \frac{u(X)}{a_1 X} = \left(\frac{X_p}{X}\right)^{j+1} \left(\frac{1-X^2}{1-X_p^2}\right)^{j/2} \quad (20)$$

and

$$Z(x) = \frac{1}{x^2} \left( \frac{p}{p_1} \right)^{\frac{j-1}{\gamma}} \cdot \begin{cases} \left[ 1 + \frac{\gamma \chi_p^2}{\sqrt{1-\chi_p^2}} \ln \left\{ \frac{1+\sqrt{1-x^2}}{x} \right\} \right]^{\frac{\gamma-1}{\gamma}} & \text{for } j=1 \\ \left[ 1 + 2 \frac{\gamma \chi_p^3}{1-\chi_p^2} \left( \frac{1+x}{x} \right) \right]^{\frac{\gamma-1}{\gamma}} & \text{for } j=2 \end{cases} \quad (21)$$

The corresponding velocity and pressure profiles can be then expressed as

$$u(x) = \left( \frac{\chi}{x} \right)^j \left( \frac{1-x^2}{1-\chi_p^2} \right)^{j/2} \chi_p a_1 \quad (22)$$

and

$$\frac{p-p_1}{p_1} = \begin{cases} \gamma \frac{\chi_p^2}{\sqrt{1-\chi_p^2}} \ln \left\{ \frac{1+\sqrt{1-x^2}}{x} \right\} & \text{for } j=1 \\ 2\gamma \frac{\chi_p^3}{1-\chi_p^2} \left( \frac{1+x}{x} \right) & \text{for } j=2 \end{cases} \quad (23)$$

The above set of equations provides a complete description of the acoustic wave in terms of a single variable  $x$ , the self-similarity coordinate, and the parameter  $\chi_p$ , equivalent to  $\zeta^{-1/2}$ , as it can be verified directly from the definitions of  $\zeta$  and  $Z_p$  by noting that, for the acoustic wave,  $\gamma = 1$  while  $a_p \approx a_1$ .

For the plane-symmetrical case ( $j = 0$ ) the acoustic wave is identical to the blast wave corresponding to  $\gamma = 1$ , one being just a simple limit of the other without any anomaly.

The flame is considered to act as a deflagration, as depicted on Fig. 2. From the analysis of the thermodynamic processes represented on this diagram, taking properly into account the dependence of the heat of reaction on the temperature immediately ahead of the flame, one obtains the relation

$$\mathcal{V}_F \equiv \frac{N_F}{N_1} = \chi_i^2 \frac{Z_i}{Z_1} \left[ \frac{1}{1-F_i} - \frac{\delta_i}{\delta_j} \frac{F_i}{Z_i} \left( 1 + \frac{\delta_i-1}{2} F_i \right) \right] - \left( 2 \frac{\delta_i}{\delta_j} \frac{\delta_i-1}{\delta_i-1} \cdot \mathcal{M} \right) \left( \chi_i^2 \frac{Z_i}{Z_1} - 1 \right) \quad (24)$$

where  $\mathcal{M} = \frac{m_i}{m_j}$  is the molecular weight ratio.

In the course of computations the parameters  $Z_i$ ,  $F_i$  and  $X_i$  are evaluated point by point starting from the piston face. The corresponding value of  $V_F$  can be therefore determined from Eq. (24) and the position of the flame front is thus established when it attains the appropriate magnitude for a given combustible mixture.

The two terms in the square brackets represent, respectively, the two components of the expression

$$V_F \equiv \frac{N_F}{N_i} = V_j + \frac{X_i}{Z_i} \frac{(1-V_j)(V_j-\beta)}{(1+\beta)V_j^2} \quad (25)$$

where  $\beta = (\delta_j - 1)/(\delta_j + 1)$  while

$$V_j = \frac{1}{1-F_i} \quad (26)$$

For a constant pressure deflagration,  $V_F = V_j$  and, consequently, the second term in the brackets vanishes. If, moreover, the influence of heating in the blast wave is negligible,  $X_i^2 \frac{Z_i}{Z_i} = \left(\frac{Q_i}{Q_i}\right)^2 \approx 1$  and Eq. (24) is reduced to the asymptotic form

$$V_F \approx V_j = \frac{1}{1-F_i} \quad (27)$$

The value of the parameter  $F = F_i$  at the flame front is, under such circumstances, established solely on the basis of the value of  $V_F$  as specified above.

Finally it should be noted that to each point of the integral curve there corresponds a certain value of the burning speed given by the relation:

$$S = X_i W_2 (1-F_i) \quad (28)$$

## RESULTS

For numerical computations, a typical case of a hydrocarbon-air mixture initially at N.T.P. conditions was used. Its thermodynamic properties were expressed in terms of the following parameters

$$\begin{array}{lll} V_F = 7 & Q_1 = 345 \text{ /sec} & \rho_1 = 1 \text{ atm} \\ \gamma_1 = \gamma_2 = \gamma_3 = 1.3 & \gamma_1 = \gamma_4 = 1.2 & M = 1 \end{array}$$

Figure 3 represents integral curves on the phase plane together with the corresponding plot of  $X=X(F)$ . Each is labeled with the appropriate value of the particular  $\zeta = \gamma Z_F$ . Points corresponding to the flame front are indicated by triangles. As pointed out before, the transition between the blast wave solution and the acoustic regime is continuous. At  $\zeta = 10^2$  the two are exactly coincident. For  $\zeta > 10^2$  the acoustic solutions become quite accurate, while the numerical computations for the blast wave get to be very lengthy and, hence, suffer from loss in accuracy.

To give a complete physical description of the flow fields thus evaluated, the corresponding particle velocity, temperature and pressure profiles for the spherical case of  $j = 2$  are presented in Figs. 4, 5 and 6, respectively.

Figure 7 gives the burning speed,  $S$ , evaluated from Eq. (28), as a function of  $V_F$  determined by the use of Eq. (24) for the spherically symmetric waves, with  $\zeta$  as the parameter. The graph is quite general in that it is applicable to any value of the heat of reaction that may be ascribed to the combustible mixture. As on the other diagrams, points corresponding to the given substance for which  $V_F = 7$  are denoted by triangles. The burning speed,  $S$ , has an upper bound given by the CJ deflagration limit. It is specified by the condition  $X_3 W_2 = Q_4$  and is represented on the diagram by the chain-dotted line.

The most significant physical parameters for all the geometries are shown in Fig. 8, plotted as a function of  $\zeta$ , the parameter identifying specific solutions. This includes the burning speed,  $S$ , and the flame position,  $x_3$ , both referring to a typical hydrocarbon-air mixture that corresponds to  $V_F = 7$ , as well as the front parameter  $\gamma = 1/M^2$ . The latter exhibits most distinctly the effect of the geometry on the strength of the wave generated by the flame -- the Mach number increasing considerably from a point- to a plane-symmetrical case for the same value of  $S$ , while the corresponding change in  $x_3$  is quite insignificant.

Finally Fig. 9 displays significant pressure levels as a function of the burning speed  $S$  attained in a combustible medium corresponding to  $V_F = 7$ . For the same burning speeds, the differences between the three geometries are quite significant, the plateau of  $p_3 = p_2$  for the plane-symmetrical wave being appreciably higher than the pressure levels in the other two cases. In practice one can expect such high pressures to be attained whenever the flame front is well confined, as in corridors or tunnels.

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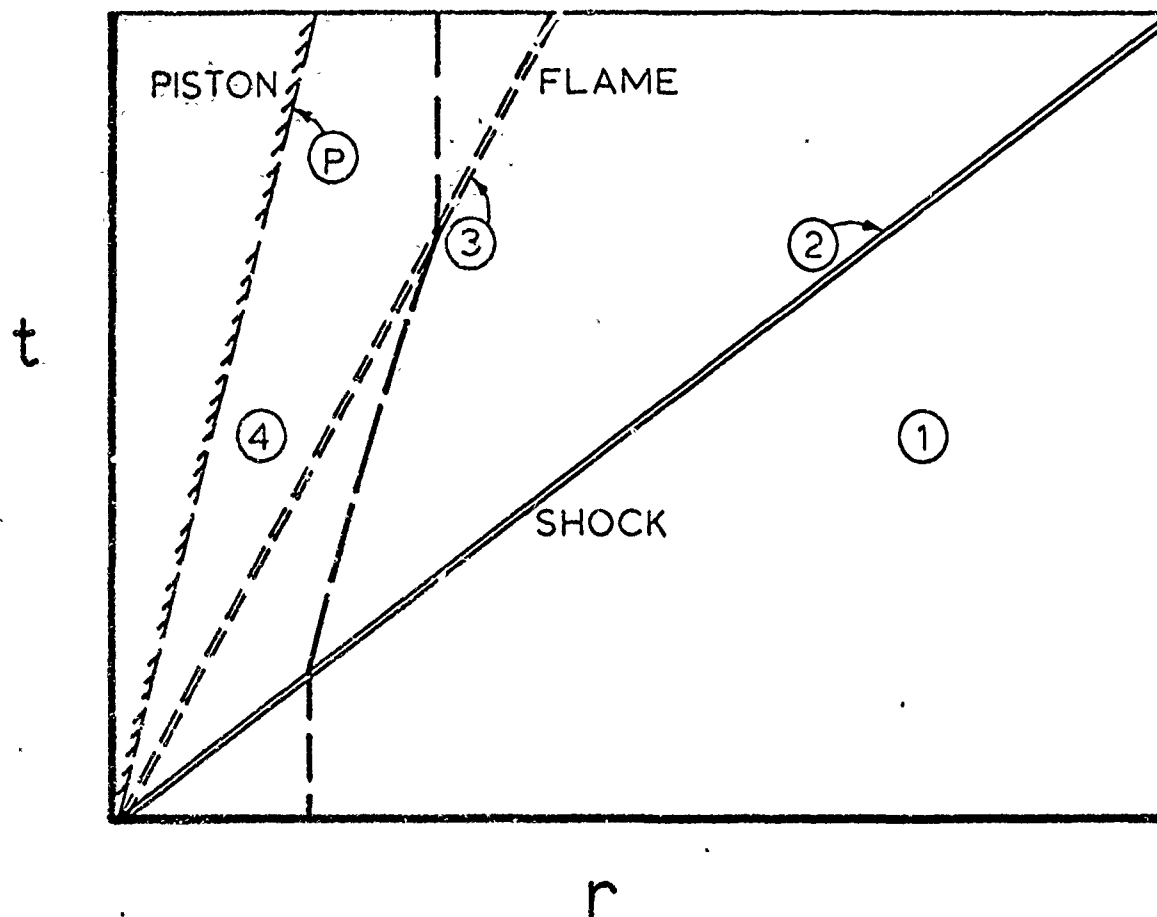


Figure 1.

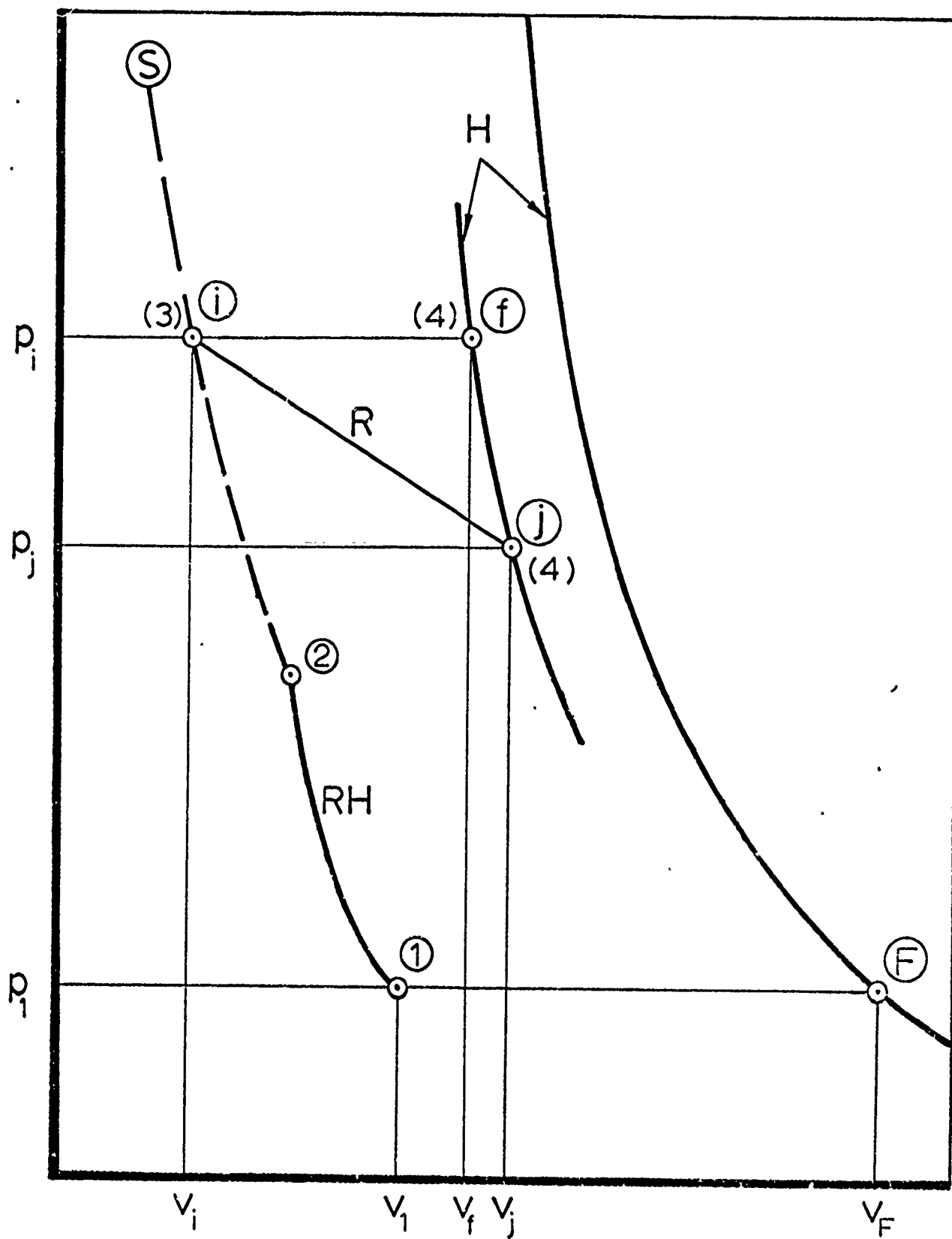


Figure 2.

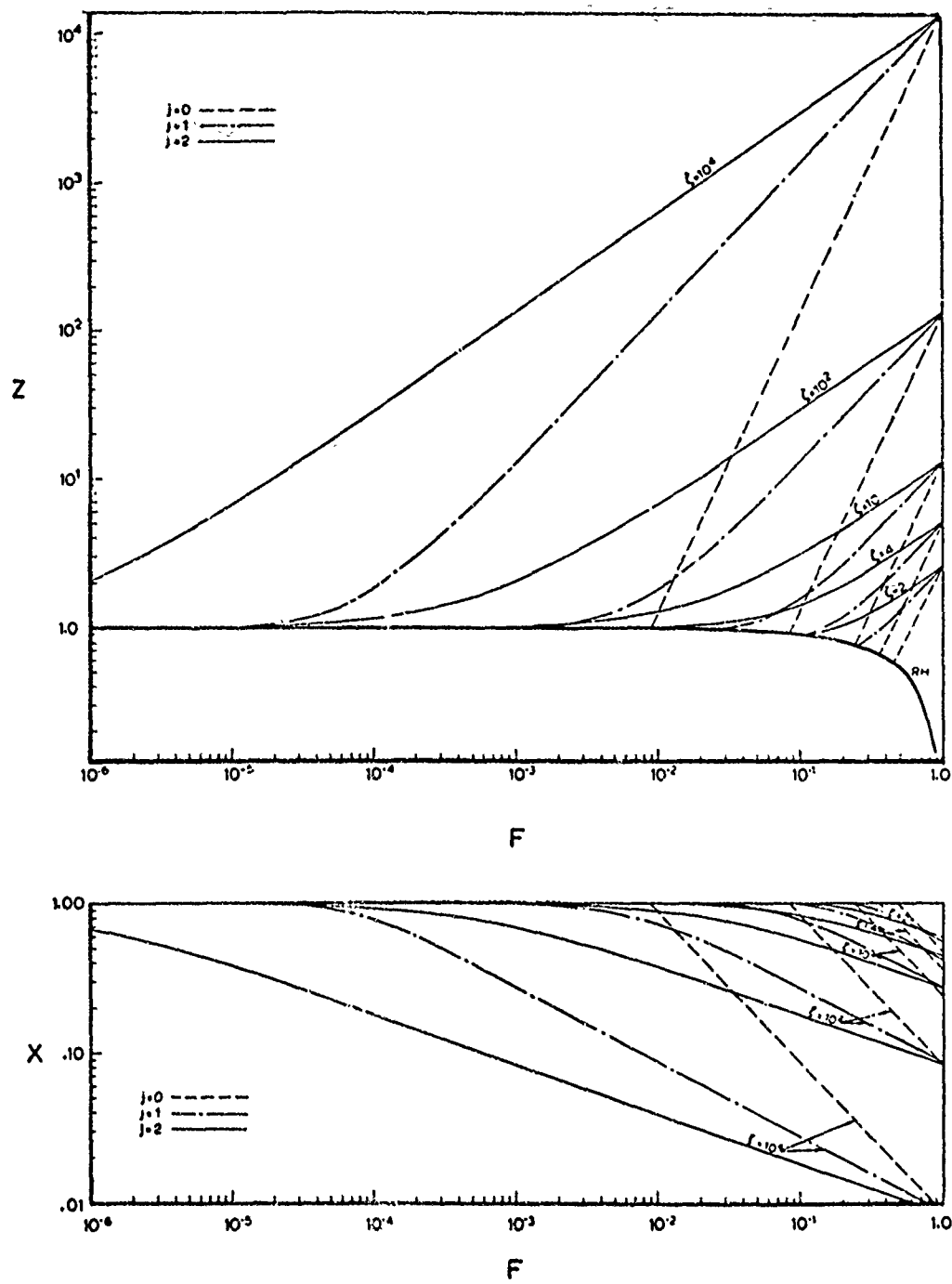


Figure 3.

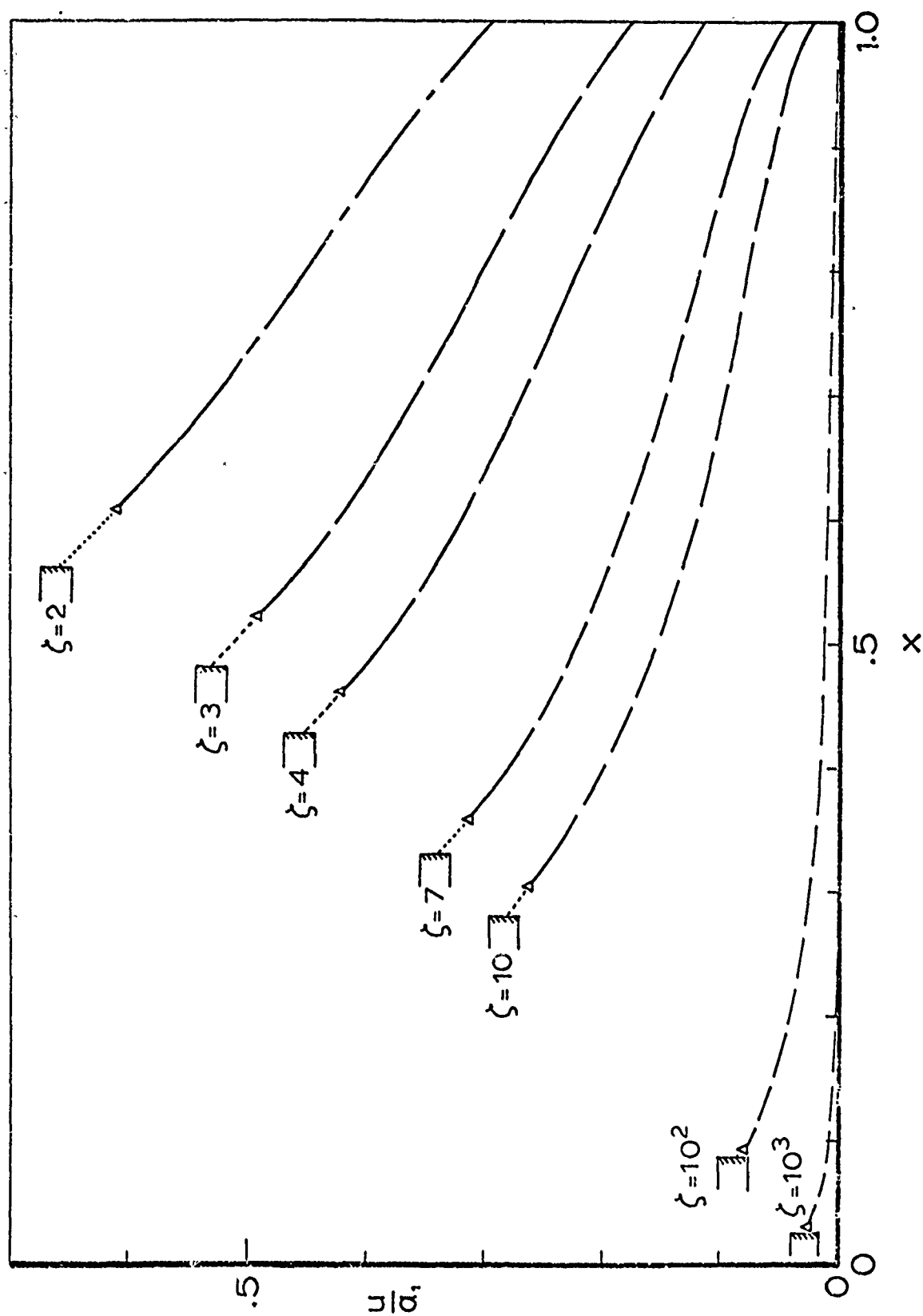


Figure 4

Figure 4

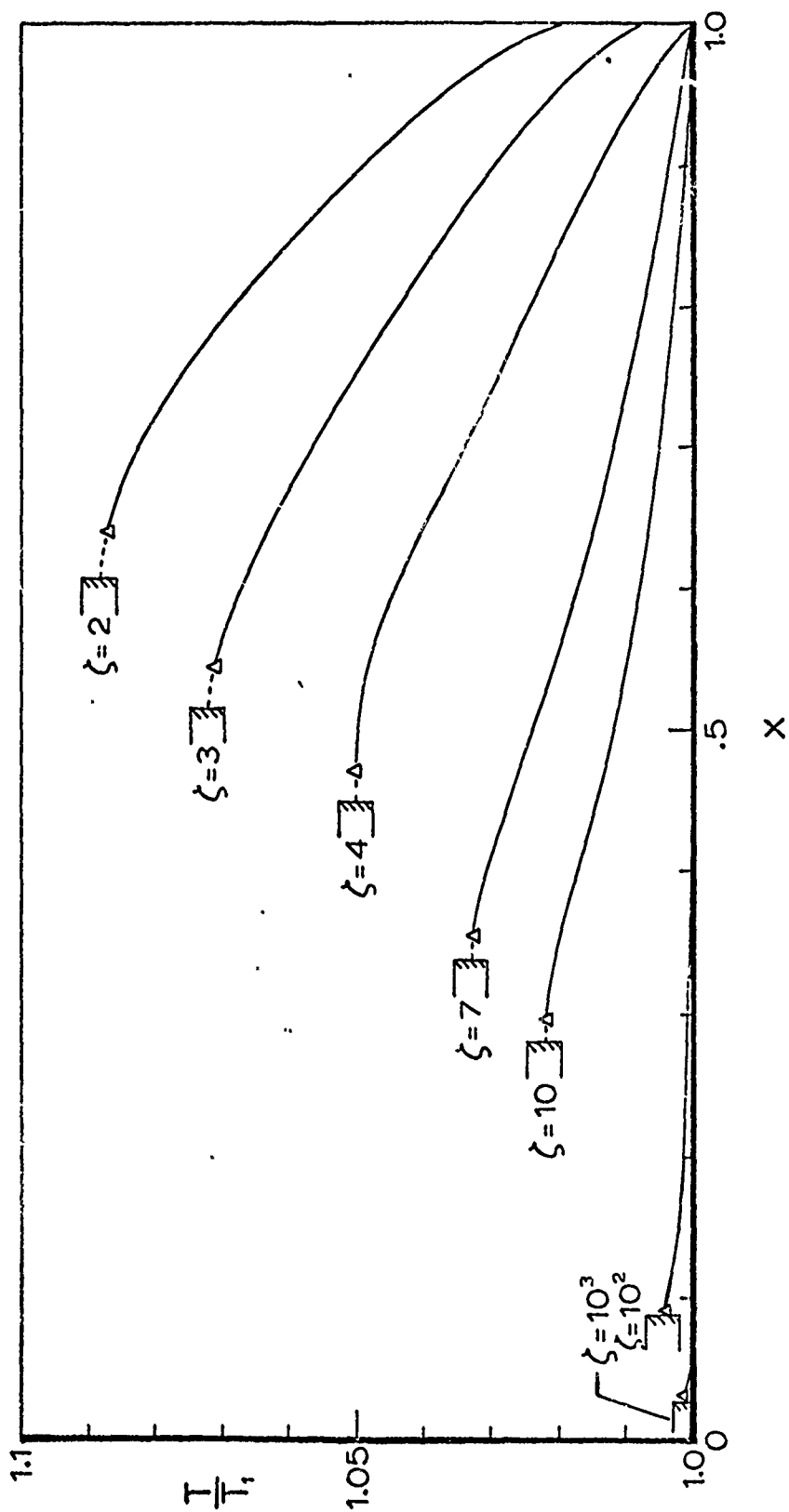


Figure 5.

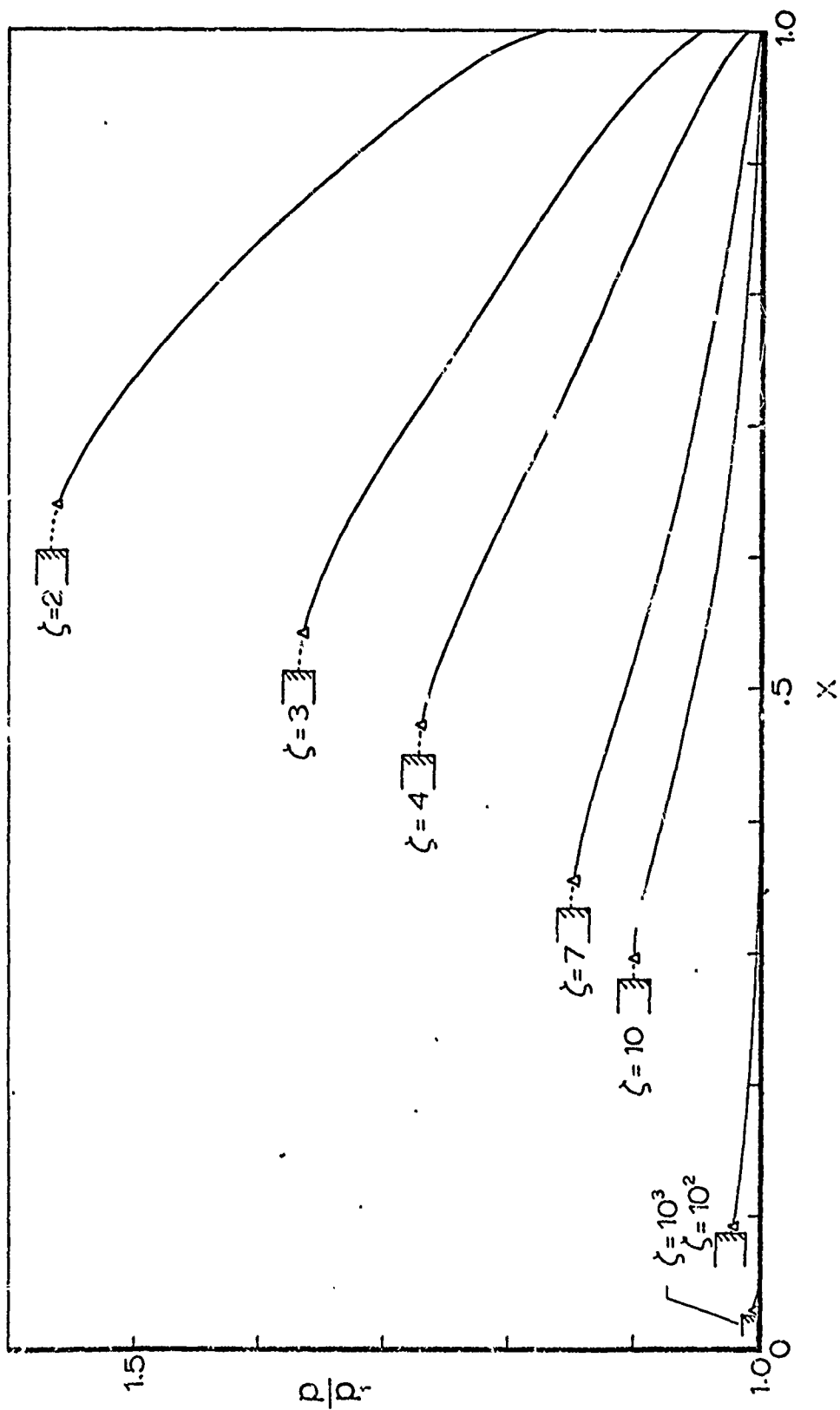


Figure 6.

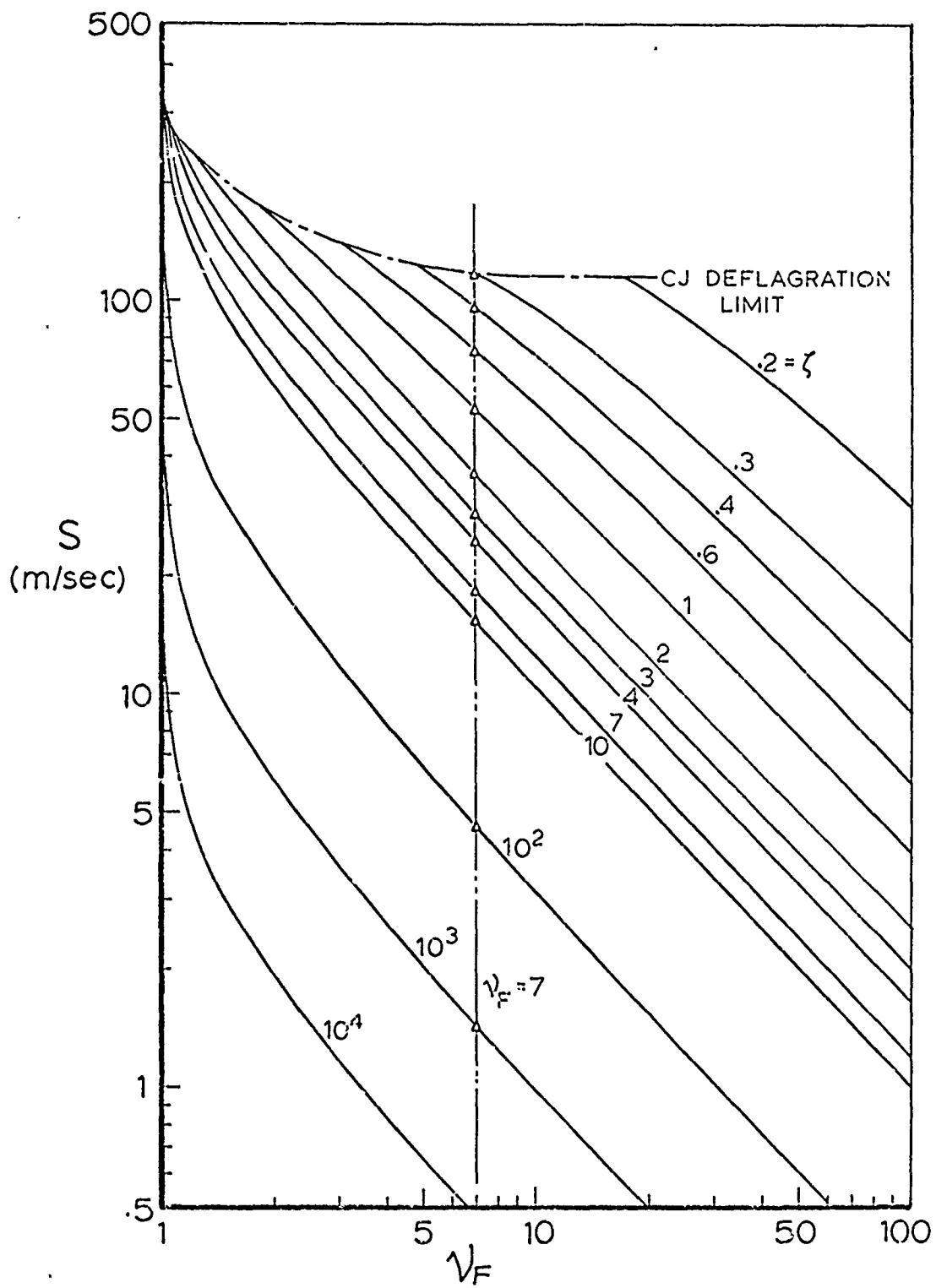


Figure 7.

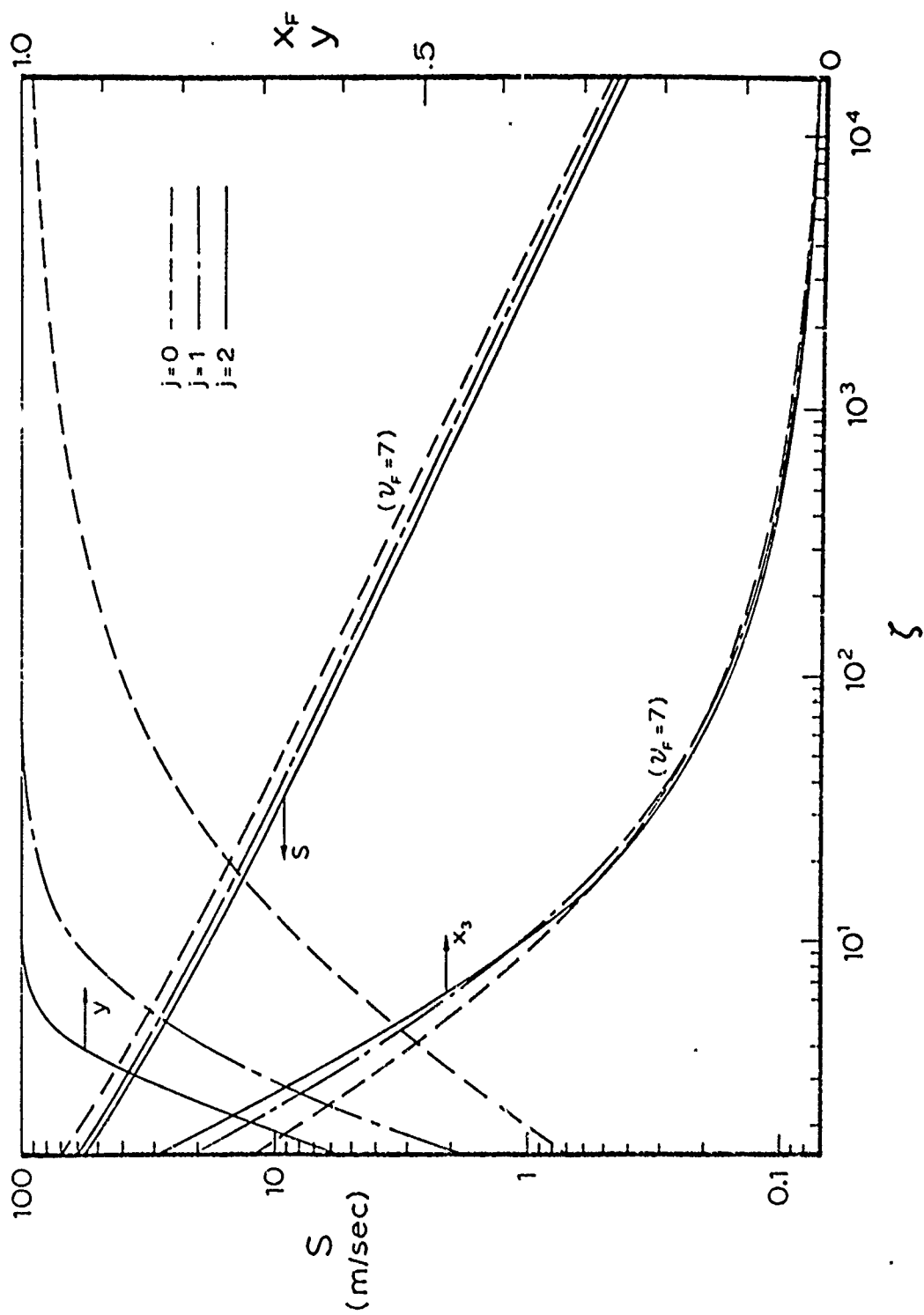


Figure 8.

$\frac{p_3}{p_1}$   
 $\frac{p_2}{p_1}$

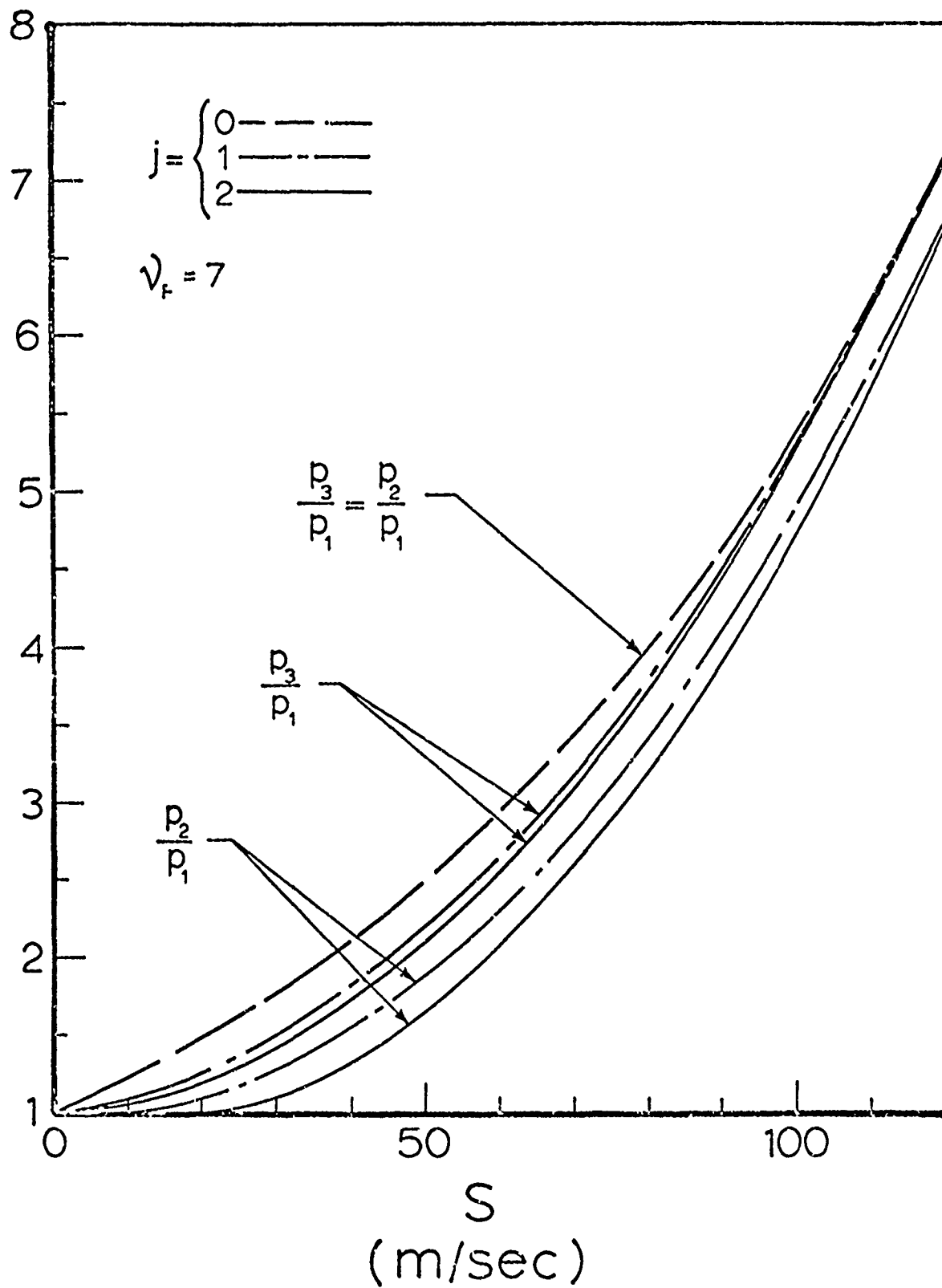


Figure 9.